Exhibit D

Assessing Model Fit with Sampling Data at Tarawa Terrace Water-Supply Wells and the Water Treatment Plant

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INTRODUCTION

In evaluating the goodness of the model fit with available sampling data for Tarawa Terrace (TT) water-supply wells and the Tarawa Terrace water treatment plant (TTWTP), Maslia et al. (2007)[1] compute the geometric bias as described in Table A8 (p. A26) for TT water-supply wells and the TTWTP. The geometric bias is defined as (Maslia et al. 2007, p. A25, Equation 1):

$$B_g = \exp\left[\frac{\sum_{i=1}^{N} ln\left(B_{m,i}\right)}{N}\right] \qquad (1),$$

where

- $B_{m,I}$ is the model bias defined as the ratio of simulated concentration to observed concentration (C_{sim} / C_{obs}),
- N is the number of sampling points,
- $ln(\,)$ is the Naperian or natural logarithm, and
- B_g is the geometric bias.

C_{sim}/C_{obs} has the following properties:

- Model underprediction for $C_{sim}/C_{obs} <1$,
- Model unbiased for $C_{sim}/C_{obs} = 1$, and
- Model overprediction for $C_{sim}/C_{obs} >1$.

In the TT Chapter A report, Maslia et al. (2007) compute the geometric bias (B_g) for TT water-supply wells as 5.8 (for all water-supply wells that have sampling data above detection limits—Table A9) and 3.9 when water-supply well TT-23 is omitted. For the TTWTP the computed geometric bias is 1.5 (for all sampling data above detection limits—Table A10). These values indicate that there is an overprediction by the model because B_g is greater than 1.0.

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[1] Maslia ML, Sautner JB, Faye RE, Suárez-Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr, and Krueger AL. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter A: Summary of Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

DUPLICATE SAMPLING DATA

Reviewing the sampling data listed in Tables A9 and A10 for TT supply wells and the TTWTP, respectively, Dr. Leonard F. Konikow has opined that when multiple sampling data for the same day or the same month occur, the duplicates should be removed from these calculations (or use an average of the duplicate samples) because the groundwater-flow and contaminant fate and transport models for TT were calibrated using a 1-month stress period (time step). He also noted that it is common practice to replace observations of non-detects with a value of one half of the detection limit (0.5*DL). Because the true value of a non-detect (ND) sample can lie between zero and the detection limit (DL), we also computed the geometric bias for a limiting case in which it is assumed that ND=DL; the difference in the computed bias for this case and the scenario assuming ND=0.5*DL would provide an indicator of the sensitivity of the calculated bias to uncertainty in the common assumption that the observed value equals half of the detection limit.

In a more general sense, imagine if one had a simulation with 24 monthly time steps (24 simulated values) and there is one field observation per month, except for one month when there are 25 observations. If all observations are used to generate residuals, the bias you obtain from the one month with 25 observations would dominate the overall bias number. However, if you average those 25 values, one obtains a much better sense of the overall model bias.

RECOMPUTING MODEL AND GEOMETRIC BIAS

Using Dr. Konikow's suggestions, the following scenarios were developed to compute updated model and geometric biases. The calculations are provided in two adjoining MS Excel files whose names are:

TT-Wells_Model Bias.xlsx, for TT supply wells and sampling data listed in Table A9, and **TT-WTP_Model Bias.xlsx**, for the TTWTP sampling data list in Table A10.
Each MS Excel file contains four worksheets for the different computed model and geometric biases listed in Table 1.

Table 1. Descriptions of scenarios for computing model and geometric bias for the Tarawa Terrace water-supply wells and water treatment plant.

[DL, detection limit; ND, non-detections]

Worksheet Name	Description
Published No NDs (Scenario 0)	Data published in the ATSDR Chapter A report, Tables A9 (TT supply wells) and Table A10 (TTWTP) and resulting geometric bias results published in Table A8. These calculations are provided to confirm the results are the same as in the published Chapter A report (all non-detections [ND] are not included in calculations because the ln[ND] is undefined)
Mean of Duplicates (Scenario 1)	Calculations conducted by taking an average (mean) of sampling data that occur within the same month (NDs are **not** included)
ND = DL, Mean of Duplicates (Scenario 2)	Calculations conducted by assigning the detection limit (DL) to the value of the non-detection (ND) sample. For multiple samples within the same month, the average (mean) of sampling data is used as per Scenario 1
ND = 0.5DL, Mean of Duplicates (Scenario 3)	Calculations conducted by assigning ½ of the detection limit (DL) to the value of the non-detection (ND) sample. For multiple samples within the same month, the average (mean) of sampling data is used as per Scenario 1

Results of the computation for model and geometric biases for the four scenarios listed in Table 1 for the TT water-supply wells and the TTWTP are listed in Table 2.

Table 2. Results of model and geometric bias computations for scenarios listed in Table 1.
[DL, detection limit; ND, non-detection]

Scenario	Description	Number of Sampling Values* (Total Sampling Points)	Computed Model Bias
Tarawa Terrace Water-Supply Wells (Table A9 in TT Chapter A)			
0	Published No NDs	19 (36)	5.8 (3.9 without TT-23)
1	Mean of Duplicates	13 (36)	3.6
2	ND = DL mean of duplicates	24 (36)	2.5
3	ND = 0.5*DL mean of duplicates	24 (36)	3.4
Tarawa Terrace Water Treatment Plant (Table A10 in TT Chapter A)			
0	Published No NDs	10 (25)	1.5
1	Mean of Duplicates	5 (25)	1.4
2	ND = DL mean of duplicates	11 (25)	0.84
3	ND = 0.5*DL mean of duplicates	11 (25)	1.3

** Number of observed values (direct or averaged) used in bias calculation. For a value to be usable, both the simulated and observed concentrations must be non-zero.*

DISCUSSION

These results indicate that by taking the means of samples that occur within the same month or by substituting specific concentration values for non-detections based on the detection limit (DL), the resulting computed model geometric biases are lower (closer to 1.0) than originally published in Table A8 (using data listed in Tables A9 and A10 in the TT Chapter A report). For the TTWTP, when the detection limit (DL) is substituted for non-detections (ND), the geometric bias falls slightly below 1.0 to 0.84, indicated a slight model underprediction. When one-half (1/2) of the detection limit (0.5*DL) is used for a non-detection, the geometric bias is just slightly above 1.0 with a value of 1.3, indicating a slight model overprediction (Table 2).

Two points are noteworthy. First, in the re-calculation of the model and geometric biases, the published simulated (reconstructed) PCE (tetrachloroethylene) concentrations for a single-specie listed in Malia et al. (2007, Appendix A2, column 3) were used and no additional simulations were conducted. Second, simulated (reconstructed) concentrations of PCE for TT supply wells and the TTWTP occur on the last day of each month (e.g., January 31, February 28 (29), . . . December 31) and represent a mean value over the entire month. Removing duplicates (by substituting a mean value for multiple samples) or substituting values for non-detections (also referred to as censored data) from analyses is a much-discussed subject. Helsel (2005) [2] discusses this in detail and provides alternative methods for using non-detection data for statistical analyses of environmental data.

[2] Helsel, D.R., 2005. Nondetects and data analysis: Statistics for Censored Environmental Data. John Wiley & Sons, Inc., 250 p.